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Positive extension problems for a class of structured matrices☆

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Abstract

We consider positive definite (semidefinite) extension problems for matrices with structure determined via a Stein equation. Some related extremal problems (maximal and minimal rank extensions, maximal determinant extension) are also considered. Connections with interpolation problems for a certain class of analytic contractive valued functions on the unit ball of $\mathbb{C}^d$ are discussed.

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1. Introduction

Let $(T_1, \ldots, T_d)$ be a d-tuple of $n \times n$ complex matrices which is stable in the sense that the spectrum of the matrix $\sum_{j=1}^{d} T_j \otimes \overline{T}_j$ sits inside the open unit disk $\mathbb{D}$. Then in particular,

$$\det\left(I_{n^2} - \sum_{j=1}^{d} T_j \otimes \overline{T}_j\right) \neq 0 \tag{1.1}$$

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and therefore, the Stein equation

$$P - T_1 P T_1^* - \cdots - T_d P T_d^* = Q \tag{1.2}$$

has a unique solution P for every choice of $Q \in \mathbb{C}^{n\times n}$ [27, Section 8.4]. Thus, if Q is hermitian, the unique solution P of (1.2) is also hermitian. We shall take Q in the form $Q = EE^* - MM^*$ where $E \in \mathbb{C}^{n\times p}$ and $M \in \mathbb{C}^{n\times q}$, and consider the generalized Stein equation

$$P - \sum_{j=1}^{d} T_j P T_j^* = EE^* - MM^*, \tag{1.3}$$

which, under assumption (1.1), has a unique solution $P = P^*$. Equations of the form (1.2) with Q positive definite were studied in [29,30]. Eqs. (1.2) with $Q \geqslant 0$ and commuting T_j's arise in characterization (see [11]) of backward shift invariant subspaces of the Arveson space that are isometrically included in this space. The Stein equation of the form (1.2) with a hermitian right-hand side part and commuting matrices T_j's appears in interpolation problems for contractive multipliers of the Arveson space [6–8].

In the present paper we consider positive definite (semidefinite) extension problems related to the Stein equation (1.3). Let

$$\widehat{T}_j = \begin{bmatrix} T_j & 0 \\ V_j & z_j I_k \end{bmatrix} \quad (j = 1, \ldots, d) \tag{1.4}$$

(I_k stands for the $k \times k$ identity matrix) be lower triangular extensions of T_j's such that the extended d-tuple $(\widehat{T}_1, \ldots, \widehat{T}_d)$ is still stable. Then, in particular,

$$\det\left(I_{(n+k)^2} - \sum_{j=1}^{d} \widehat{T}_j \otimes \overline{\widehat{T}}_j\right) \neq 0, \tag{1.5}$$

which clearly reduces to three conditions, one of which is (1.1) and the other two of which are

$$1 - \sum_{j=1}^{d} |z_j|^2 \neq 0 \quad \text{and} \quad \det\left(I_n - \sum_{j=1}^{d} z_j T_j^*\right) \neq 0.$$

Since the d-tuple $(\widehat{T}_1, \ldots, \widehat{T}_d)$ is stable, we have, in fact, $1 - \sum_{j=1}^{d} |z_j|^2 > 0$. In other words we assume that the point $z = (z_1, \ldots, z_d)$ belongs to the unit ball

$$\mathbb{B}^d = \left\{ z = (z_1, \ldots, z_d) : \sum_{j=1}^{d} |z_j|^2 < 1 \right\}$$

of $\mathbb{C}^d$ and that the matrix

$$G(z) := I_n - \sum_{j=1}^{d} z_j T_j^* \tag{1.6}$$

is invertible. Under assumption (1.5), the extended Stein equation

$$\widehat{P} - \sum_{j=1}^{d} \widehat{T}_j \widehat{P} \widehat{T}_j^* = \widehat{E}\widehat{E}^* - \widehat{M}\widehat{M}^* \tag{1.7}$$

has a unique solution $\widehat{P}$ for every choice of the matrices $\widehat{E}$ and $\widehat{M}$ on its right-hand side. We choose these matrices to be extensions of E and M respectively, i.e., to be of the form

$$\widehat{E} = \begin{bmatrix} E \\ \mathbf{e} \end{bmatrix} \quad \text{and} \quad \widehat{M} = \begin{bmatrix} M \\ x \end{bmatrix}, \tag{1.8}$$

where $\mathbf{e} \in \mathbb{C}^{k\times p}$ is fixed and $x \in \mathbb{C}^{k\times q}$ is a variable. Then the unique solution $\widehat{P} = \widehat{P}_x$ of the extended Stein equation (1.7) depends on x. A comparison of the top principal blocks in (1.7) leads us to the conclusion that the top principal block of $\widehat{P}$ satisfies (1.3), and therefore equals P, since (1.3) has a unique solution. Therefore, necessarily $\widehat{P}$ is of the form

$$\widehat{P}_x = \begin{bmatrix} P & \beta^* \\ \beta & \gamma \end{bmatrix}, \quad \gamma \in \mathbb{C}^{k\times k}, \quad \beta \in \mathbb{C}^{k\times n}, \tag{1.9}$$

i.e., it extends P, which suggests the following extension problem:

Problem 1.1. Given a stable d-tuple $(\widehat{T}_1, \ldots, \widehat{T}_d)$ of $(n+k)\times(n+k)$ matrices of the form (1.4), given $\widehat{E} \in \mathbb{C}^{(n+k)\times p}$ and $M \in \mathbb{C}^{n\times q}$, find all matrices $x \in \mathbb{C}^{k\times q}$ such that the unique solution $\widehat{P}_x$ of the extended Stein equation (1.7) is positive semidefinite.

It is well known that many classes of structured matrices can be defined via matrix equations: if the rank of the matrix $EE^* - MM^*$ is small relative to n, the entries of a unique solution P of the Stein equation (1.3) depend on a relatively small number of parameters; in other words, P is of a certain structure. The requirement that $\widehat{P}$ satisfies the extended Stein equation (1.7) means that we extend P while preserving this structure. Thus, for special choices of $\widehat{T}_j$'s, E and M, Problem 1.1 reduces to various structured positive semidefinite extension problems.

Let us give a somewhat different interpretation of Problem 1.1, starting with $\widehat{P}$ rather than with P. Let $\widehat{P}$ satisfy the extended Stein equation (1.7) and let (1.9) be its block decomposition conformal with decompositions (1.8) and (1.4). Upon substituting (1.4), (1.9) and (1.8) into the matrix identity (1.7) and comparing the corresponding block entries, we come to the three equalities, the first of which coincides with (1.3) and the remaining two of which are

$$\beta - \sum_{j=1}^{d} V_j P T_j^* - \sum_{j=1}^{d} z_j \beta T_j^* = \mathbf{e}E^* - xM^*,$$

$$\gamma - \sum_{j=1}^{d}(V_j P V_j^* + z_j \beta V_j^* + V_j \beta^* \bar{z}_j + |z_j|^2\gamma) = \mathbf{e}\mathbf{e}^* - xx^*,$$

and imply

$$\beta = \left(\mathbf{e}E^* - xM^* + \sum_{j=1}^{d} V_j P T_j^*\right) G(z)^{-1}, \tag{1.10}$$

$$\gamma = \frac{1}{1-|z|^2}\left(\mathbf{e}\mathbf{e}^* - xx^* + \sum_{j=1}^{d}(V_j P V_j^* + z_j \beta V_j^* + V_j \beta^* \bar{z}_j)\right), \tag{1.11}$$

where $G(z)$ is given by (1.6) and where $|z|^2 := \sum_{j=1}^{d} |z_j|^2$. Now we relax the stability assumption on $(\widehat{T}_1, \ldots, \widehat{T}_d)$ to

$$\sum_{j=1}^{d} |z_j|^2 < 1 \quad \text{and} \quad \det\left(I_n - \sum_{j=1}^{d} z_j T_j^*\right) \neq 0. \tag{1.12}$$

These two latter conditions do not guarantee that the Stein identity (1.3) defines the block P in $\widehat{P}$ uniquely. However, if one fixes this block along with $\widehat{T}_j$'s, $\widehat{E}$ and M, then the block entries β and γ in $\widehat{P}$ will depend on the variable x only, which is easily seen from formulas (1.10) and (1.11). Thus, if P satisfies the Stein identity (1.3), then for every $x \in \mathbb{C}^{k\times q}$, the extended Stein equation (1.7) has a unique solution $\widehat{P}_x$ of the form (1.9). This suggests the following problem which is more general than Problem 1.1 and which reduces to that problem under additional stability conditions on the matrices T_j's.

Problem 1.2. Given matrices $\widehat{T}_1, \ldots, \widehat{T}_d$ of the form (1.4) and satisfying conditions (1.12), given matrices $P \in \mathbb{C}^{n\times n}$, $\widehat{E} \in \mathbb{C}^{(n+k)\times p}$ and $M \in \mathbb{C}^{n\times q}$, find all matrices $x \in \mathbb{C}^{k\times q}$ such that the unique extension $\widehat{P}_x = \begin{bmatrix} P & * \\ * & * \end{bmatrix}$ of P satisfying the extended Stein equation (1.7) is positive semidefinite.

Strictly speaking, Problem 1.2 is a positive semidefinite *completion* problem, since we are asked to complete a partially specified matrix $\widehat{P}$, subject to the Stein identity (1.7), to a fully specified positive semidefinite matrix. However, as the specified pattern P in $\widehat{P}$ is its principal submatrix, we still refer to this problem as to an extension problem.

It is clear from the preceding analysis that conditions

$$P \geqslant 0 \quad \text{and} \quad P - \sum_{j=1}^{d} T_j P T_j^* = EE^* - MM^* \tag{1.13}$$

are necessary for Problem 1.2 to have a solution. In Section 2 we shall show that these conditions are also sufficient and we shall describe the set of all solutions of Problem 1.2 when these conditions are met. A problem related to Problem 1.2 is

Problem 1.3. Given the data as in Problem 1.2, find all matrices $x \in \mathbb{C}^{k\times q}$ such that the unique extension $\widehat{P}_x = \begin{bmatrix} P & * \\ * & * \end{bmatrix}$ of P satisfying the extended Stein equation (1.7) is positive definite.

Obvious necessary conditions for this problem to have a solution are

$$P > 0 \quad \text{and} \quad P - \sum_{j=1}^{d} T_j P T_j^* = EE^* - MM^*.$$

The next example shows that these condition are not sufficient.

Example 1.4. Let $T_j = 0_{n\times n}$ for $j = 1, \ldots, d$ and let $E = I_n$ and $M = 0_{n\times q}$. Then $P = I_n > 0$ is the unique solution of the Stein equation (1.3). Furthermore, let $\mathbf{e} = 0_{k\times p}$ and let $\widehat{T}_j = 0_{(n+k)\times(n+k)}$ for $j = 1, \ldots, d$. Then for every choice of $x \in \mathbb{C}^{k\times q}$, the unique solution $\widehat{P}_x$ of the extended Stein equation (1.7) is of the form

$$\widehat{P}_x = \widehat{E}\widehat{E}^* - \widehat{M}\widehat{M}^* \in \mathbb{C}^{(n+k)\times(n+k)}$$

and cannot be positive definite, since it has not more than n positive eigenvalues.

Necessary and sufficient conditions for Problem 1.3 to have a solution will be presented in Section 4.

For the case when $d = 1$, Problems 1.3 and 1.2 were considered in [14] and [9], respectively. The results presented in Sections 2 and 3 generalize some results from the referred papers to the case when $d > 1$. The standard treatment of positive definite extension problems involves the Schur complement and is based on a simple fact that.

Remark 1.5. A block matrix $\widehat{P}$ of the form (1.9) is positive definite if and only if $P > 0$ and the matrix $\gamma - \beta P^{-1}\beta^*$ (the Schur complement of P in $\widehat{P}$) is positive definite.

Upon making use of formulas (1.10) and (1.11), one can express the inequality $\gamma - \beta P^{-1}\beta^* > 0$ in terms of x. Straightforward calculations then show that the set of all x satisfying this inequality form a matrix ball, and the only difficult part is to show that the semiradii of this ball are positive semidefinite (i.e., that this matrix ball is not empty). Moreover, it turns out that as in the case when $d = 1$ (considered in [14,16]), the center x_0 of this matrix ball leads to the extension $\widehat{P}_{x_0}$ of P with the maximal determinant. Using this direct approach, some partial results concerning

Problem 1.3 were obtained in [28]. Now we explain why this approach does not work so nicely for Problem 1.2.

A positive semidefinite analogue of Remark 1.5 is the following well known result, which can be found in many sources (see e.g., [13, Lemma 1.1.8]). Here and throughout the paper $A^{[-1]}$ stands for the Moore–Penrose generalized inverse of a square matrix A.

Lemma 1.6. *The following are equivalent*:

1. *The matrix* $\begin{bmatrix} P & \beta^* \\ \beta & \gamma \end{bmatrix}$ *is positive semidefinite*.
2. *It holds that*
$$P \geqslant 0, \quad \operatorname{Ker} P \subseteq \operatorname{Ker} \beta, \quad \gamma - \beta P^{[-1]} \beta^* \geqslant 0.$$
3. *It holds that*
$$P \geqslant 0, \quad \gamma \geqslant 0 \quad \textit{and} \quad \beta = \gamma^{\frac{1}{2}} S P^{\frac{1}{2}}$$
for some contractive matrix S.

It turns out to be quite difficult to satisfy the two conditions
$$\operatorname{Ker} P \subseteq \operatorname{Ker} \beta \quad \text{and} \quad \gamma - \beta P^{[-1]} \beta^* \geqslant 0 \tag{1.14}$$
simultaneously. This is the main obstruction to applying Lemma 1.6 toward solving Problem 1.2. For the case when $d = 1$, however, it was done in [9] upon taking advantage of an interpolation interpretation of the extension problem and the extensive use of results on degenerate interpolation for contractive valued analytic functions (that is, matrix-valued Schur functions). The existing results on degenerate interpolation in the d-variable setting [4] do not allow us to extend the approach from [9] to the case when $d > 1$. In this paper we present a purely algebraic solution of Problem 1.2 based on a less standard usage of Schur complement arguments. A similar trick has been used in [8] and originates in [3]. Roughly speaking, the matrix $\widehat{P}_x$ will be replaced by another matrix which is positive semidefinite if and only if $\widehat{P}_x \geqslant 0$, but for which conditions similar to those in (1.14) can be verified easily. This will be done in Lemma 2.3, the main technical result of the paper. Using this result, we shall treat some extremal problems related to Problems 1.2 and 1.3 in Sections 3 and 5.

In Section 6 we shall also consider an extension problem of a different type. In that new setting $\mathbf{e}$ and x will be matrix-valued functions of the variable $z = (z_1, \ldots, z_d)$ defined on the unit ball $\mathbb{B}^d$, whereas $\widehat{T}_j$, $\widehat{E}$ and $\widehat{M}$ will be the matrix-valued functions defined by
$$\widehat{T}_j(z) = \begin{bmatrix} T_j & 0 \\ 0 & z_j I_k \end{bmatrix} \quad (j = 1, \ldots, d), \tag{1.15}$$
$$\widehat{E}(z) = \begin{bmatrix} E \\ \mathbf{e}(z) \end{bmatrix} \quad \text{and} \quad \widehat{M}(z) = \begin{bmatrix} M \\ x(z) \end{bmatrix}. \tag{1.16}$$

It turns out (see Section 6), that if P is any solution to the Stein identity (1.3), then there exists a unique extension $\widehat{P} = \widehat{P}_x(z, w)$ of P, satisfying the extended functional Stein equation

$$\widehat{P} - \sum_{j=1}^{d} \widehat{T}_j(z)\widehat{P}\,\widehat{T}_j(w)^* = \widehat{E}(z)\widehat{E}(w)^* - \widehat{M}(z)\widehat{M}(w)^*. \tag{1.17}$$

Moreover, it turns out that $\widehat{P}_x(z, w)$ is a matrix-valued function of two variables $z, w \in \mathbb{B}^d$ of the form

$$\widehat{P}_x(z, w) = \begin{bmatrix} P & \beta(w)^* \\ \beta(z) & \gamma(z, w) \end{bmatrix}$$

(explicit formulas for $\beta(z)$ and $\gamma(z, w)$ will be given in Section 6).

Problem 1.7. Given matrices $T_1, \ldots, T_d$ such that

$$\det\left(I_n - \sum_{j=1}^{d} z_j T_j^*\right) \not\equiv 0,$$

given matrices P, E, M, and given a $\mathbb{C}^{k\times q}$-valued function $\mathbf{e}(z)$, find all $\mathbb{C}^{k\times q}$-valued functions $x(z)$ such that the unique extension $\widehat{P}_x(z, w)$ of P satisfying the extended Stein identity (1.17) is a positive definite kernel on $\mathbb{B}^d \times \mathbb{B}^d$.

We call an $n \times n$ matrix-valued function $K(z, w)$ defined on the product set $\Omega \times \Omega$ a *positive kernel* (although it would be more precise to call it positive semidefinite) if the block matrix $[K(z_i, z_j)]_{i,j=1}^r$ is positive semidefinite for every choice of an integer r and of points $z_1, \ldots, z_r \in \Omega$. This property of K will be denoted by $K(z, w) \succeq 0$.

Some connections between Problem 1.7 and interpolation problems for a class of contractive valued analytic functions on the ball $\mathbb{B}^d$ will be discussed in Section 7.

2. Positive semidefinite extensions

In this section we shall show that under the assumption that P is a positive semidefinite solution of the Stein equation (1.3), all the solutions x of Problem 1.2 form a nonempty matrix ball, which will imply, in particular, that the necessary conditions (1.13) are also sufficient for Problem 1.2 to have a solution.

We start with some preliminaries. First we introduce the matrices

$$V = \begin{bmatrix} V_1 & \cdots & V_d \end{bmatrix}, \quad \mathbf{T} = \begin{bmatrix} T_1 & \cdots & T_d \end{bmatrix}, \tag{2.1}$$

$$Z(z) = \begin{bmatrix} z_1 I_n & \cdots & z_d I_n \end{bmatrix} \quad \text{and} \quad \mathbb{P} = \begin{bmatrix} P & & 0 \\ & \ddots & \\ 0 & & P \end{bmatrix} \in \mathbb{C}^{nd\times nd}, \tag{2.2}$$

constructed from the entries of the equation (1.3), which allow us to rewrite formulas (1.3), (1.6), (1.10) and (1.11) in a more compact form as

$$P - \mathbf{T}\mathbb{P}\mathbf{T}^* = EE^* - MM^*, \tag{2.3}$$

$$G(z) = I - Z(z)\mathbf{T}^*, \tag{2.4}$$

$$\beta = (\mathbf{e}E^* - xM^* + V\mathbb{P}\mathbf{T}^*)G(z)^{-1}, \tag{2.5}$$

$$\gamma = \frac{1}{1-|z|^2}(\mathbf{e}\mathbf{e}^* - xx^* + V\mathbb{P}V^* + \beta Z(z)V^* + VZ(z)^*\beta^*), \tag{2.6}$$

respectively. Furthermore, let us introduce the matrix

$$\widetilde{P}_x = Q(z)\widehat{P}_x Q(z)^*, \quad \text{where } Q(z) = \begin{bmatrix} \frac{G(z)^*}{\sqrt{1-|z|^2}} & 0 \\ -\frac{VZ(z)^*}{\sqrt{1-|z|^2}} & \sqrt{1-|z|^2}I_k \end{bmatrix}. \tag{2.7}$$

Remark 2.1. Since the matrix $Q(z)$ is invertible, it follows that $\widehat{P}_x \geqslant 0$ if and only if $\widetilde{P}_x \geqslant 0$.

By (1.9) and (2.7), $\widetilde{P}_x$ is of the form

$$\widetilde{P}_x = \begin{bmatrix} \frac{G(z)^*PG(z)}{1-|z|^2} & \tilde{\beta}^* \\ \tilde{\beta} & \tilde{\gamma} \end{bmatrix}, \tag{2.8}$$

where

$$\tilde{\beta} = \beta G(z) - \frac{1}{1-|z|^2}VZ(z)^*PG(z),$$

$$\tilde{\gamma} = (1-|z|^2)\gamma - VZ(z)^*\beta^* - \beta Z(z)V^* + \frac{VZ(z)^*PZ(z)V^*}{1-|z|^2}.$$

Substituting explicit formulas (2.5) and (2.6) into the two last relations and taking into account the equality

$$Z(z)^*P = \mathbb{P}Z(z)^*, \tag{2.9}$$

we come to

$$\tilde{\beta} = -xM^* + \mathbf{e}E^* + V\mathbb{P}\left(\mathbf{T}^* - \frac{Z(z)^*G(z)}{1-|z|^2}\right), \tag{2.10}$$

$$\tilde{\gamma} = \mathbf{e}\mathbf{e}^* - xx^* + V\mathbb{P}V^* + \frac{1}{1-|z|^2}VZ(z)^*PZ(z)V^*. \tag{2.11}$$

The two last formulas suggest introducing the matrices

$$\mathbf{B} = \left(\mathbf{T} - \frac{G(z)^*Z(z)}{1-|z|^2}\right)(I - Z(z)^*Z(z))^{\frac{1}{2}} \tag{2.12}$$

and

$$D = V\mathbb{P}^{\frac{1}{2}}\left(I + \frac{Z(z)^*Z(z)}{1-|z|^2}\right)^{\frac{1}{2}}. \tag{2.13}$$

The next lemma establishes important relations between these matrices.

Lemma 2.2. *Let* $\mathbf{B}$ *and* D *be given by* (2.12) *and* (2.13). *Then*

$$\mathbf{B}\mathbb{P}\mathbf{B}^* = \frac{1}{1-|z|^2}G(z)^*PG(z) - EE^* + MM^*, \tag{2.14}$$

$$DD^* = V\mathbb{P}V^* + \frac{1}{1-|z|^2}VZ(z)^*PZ(z)V^*, \tag{2.15}$$

$$D\mathbb{P}^{\frac{1}{2}}\mathbf{B}^* = V\mathbb{P}\left(\mathbf{T}^* - \frac{Z(z)^*G(z)}{1-|z|^2}\right). \tag{2.16}$$

Proof. Since

$$(I - Z(z)^*Z(z))^{\frac{1}{2}}\mathbb{P}(I - Z(z)^*Z(z))^{\frac{1}{2}} = (I - Z(z)^*Z(z))\mathbb{P},$$

it follows from (2.12) that

$$\mathbf{B}\mathbb{P}\mathbf{B}^* = \left(\mathbf{T} - \frac{G(z)^*Z(z)}{1-|z|^2}\right)(I - Z(z)^*Z(z))\mathbb{P}\left(\mathbf{T}^* - \frac{Z(z)^*G(z)}{1-|z|^2}\right).$$

Furthermore, in view of (2.9), (2.4) and by

$$Z(z)Z(z)^* = |z|^2 I_n,$$

it follows that

$$\begin{aligned}\left(\mathbf{T} - \frac{G(z)^*Z(z)}{1-|z|^2}\right)(I - Z(z)^*Z(z)) &= \mathbf{T}(I - Z(z)^*Z(z)) - G(z)^* \\ &= \mathbf{T} - Z(z)\end{aligned}$$

and thus,

$$\begin{aligned}\mathbf{B}\mathbb{P}\mathbf{B}^* &= (\mathbf{T} - Z(z))\,\mathbb{P}\left(\mathbf{T}^* - \frac{Z(z)^*G(z)}{1-|z|^2}\right) \\ &= \mathbf{T}\mathbb{P}\mathbf{T}^* - PZ(z)\mathbf{T}^* - \frac{\mathbf{T}Z(z)^*PG(z)}{1-|z|^2} + \frac{|z|^2}{1-|z|^2}PG(z) \\ &= \mathbf{T}\mathbb{P}\mathbf{T}^* - P(I - G(z)) - \frac{(I - G(z)^*)PG(z)}{1-|z|^2} + \frac{|z|^2}{1-|z|^2}PG(z) \\ &= \mathbf{T}\mathbb{P}\mathbf{T}^* - P + \frac{1}{1-|z|^2}G(z)^*PG(z),\end{aligned}$$

which implies (2.14), on account of (2.3).

Relation (2.15) follows from definition (2.13), by (2.9). Finally, since

$$(I - Z(z)^*Z(z))^{-1} = I + \frac{Z(z)^*Z(z)}{1-|z|^2},$$

it follows that

$$\begin{aligned} D\mathbb{P}^{\frac{1}{2}}\mathbf{B}^* &= V\mathbb{P}^{\frac{1}{2}}\left(I + \frac{Z(z)^*Z(z)}{1-|z|^2}\right)^{\frac{1}{2}}\mathbb{P}^{\frac{1}{2}}(I - Z(z)^*Z(z))^{\frac{1}{2}}\left(\mathbf{T}^* - \frac{Z(z)^*G(z)}{1-|z|^2}\right) \\ &= V\mathbb{P}\left(\mathbf{T}^* - \frac{Z(z)^*G(z)}{1-|z|^2}\right), \end{aligned}$$

which proves (2.16). □

Equality (2.14) suggests introducing the matrix

$$\Delta = \frac{1}{1-|z|^2}G(z)^*PG(z) + MM^* = \mathbf{B}\mathbb{P}\mathbf{B}^* + EE^*, \tag{2.17}$$

while relations (2.15), (2.16) allow us to rewrite formulas (2.10), (2.11) as

$$\tilde{\beta} = -xM^* + \mathbf{e}E^* + D\mathbb{P}^{\frac{1}{2}}\mathbf{B}^*, \quad \tilde{\gamma} = \mathbf{e}\mathbf{e}^* + DD^* - xx^*$$

and thus Problem 1.2 reduces to finding all matrices x such that

$$\widetilde{P}_x = \begin{bmatrix} \Delta - MM^* & -Mx^* + E\mathbf{e}^* + \mathbf{B}\mathbb{P}^{\frac{1}{2}}D^* \\ -xM^* + \mathbf{e}E^* + D\mathbb{P}^{\frac{1}{2}}\mathbf{B}^* & \mathbf{e}\mathbf{e}^* + DD^* - xx^* \end{bmatrix} \geqslant 0. \tag{2.18}$$

Lemma 2.3. *The matrix $\widehat{P}_x$ is positive semidefinite if and only if the following matrix is positive semidefinite*:

$$K_x = \begin{bmatrix} I_q - M^*\Delta^{[-1]}M & x^* - M^*\Delta^{[-1]}\begin{bmatrix}\mathbf{B}\mathbb{P}^{\frac{1}{2}} & E\end{bmatrix}\begin{bmatrix}D^* \\ \mathbf{e}^*\end{bmatrix} \\ x - \begin{bmatrix}D & \mathbf{e}\end{bmatrix}\begin{bmatrix}\mathbb{P}^{\frac{1}{2}}\mathbf{B}^* \\ E^*\end{bmatrix}\Delta^{[-1]}M & \begin{bmatrix}D & \mathbf{e}\end{bmatrix}\mathbf{P}_{\mathrm{Ker}[\mathbf{B}\mathbb{P}^{\frac{1}{2}}\,E]}\begin{bmatrix}D^* \\ \mathbf{e}^*\end{bmatrix} \end{bmatrix} \geqslant 0, \tag{2.19}$$

where $\mathbf{P}_{\mathrm{Ker}[\mathbf{B}\mathbb{P}^{\frac{1}{2}}\,E]}$ denotes the orthogonal projection of $\mathbb{C}^{dn+p}$ onto the kernel of the operator $\begin{bmatrix}\mathbf{B}\mathbb{P}^{\frac{1}{2}} & E\end{bmatrix}$ and where $\Delta^{[-1]}$ stands for the Moore–Penrose generalized inverse of the positive semidefinite matrix Δ given by (2.17). *Moreover*,

$$\operatorname{rank}\widehat{P}_x = \operatorname{rank}\Delta + \operatorname{rank}K_x - q \tag{2.20}$$

and

$$\det\widehat{P}_x = \frac{\det\Delta\cdot\det K_x}{|\det G(z)|^2}(1-|z|^2)^{n-k}. \tag{2.21}$$

Proof. First, we note that for every matrix S, it holds that

$$\mathbf{P}_{\mathrm{Ker}\,S} = I - S^*(SS^*)^{[-1]}S.$$

By (2.17),

$$\Delta = \begin{bmatrix} \mathbf{B}\mathbb{P}^{\frac{1}{2}} & E \end{bmatrix} \begin{bmatrix} \mathbb{P}^{\frac{1}{2}}\mathbf{B}^* \\ E^* \end{bmatrix},$$

and therefore,

$$\mathbf{P}_{\mathrm{Ker}[\mathbf{B}\mathbb{P}^{\frac{1}{2}}\,E]} = I_{dn+p} - \begin{bmatrix} \mathbb{P}^{\frac{1}{2}}\mathbf{B}^* \\ E^* \end{bmatrix} \Delta^{[-1]} \begin{bmatrix} \mathbf{B}\mathbb{P}^{\frac{1}{2}} & E \end{bmatrix}. \tag{2.22}$$

Consider the matrix

$$F_x = \begin{bmatrix} \Delta & M & \mathbf{B}\mathbb{P}^{\frac{1}{2}}D^* + E\mathbf{e}^* \\ M^* & I_q & x^* \\ D\mathbb{P}^{\frac{1}{2}}\mathbf{B}^* + \mathbf{e}E^* & x & \mathbf{e}\mathbf{e}^* + DD^* \end{bmatrix}. \tag{2.23}$$

The Schur complement of the block I_q in this matrix is equal to

$$\begin{bmatrix} \Delta & \mathbf{B}\mathbb{P}^{\frac{1}{2}}D^* + E\mathbf{e}^* \\ D\mathbb{P}^{\frac{1}{2}}\mathbf{B}^* + \mathbf{e}E^* & \mathbf{e}\mathbf{e}^* + DD^* \end{bmatrix} - \begin{bmatrix} M \\ x \end{bmatrix} \begin{bmatrix} M^* & x^* \end{bmatrix},$$

which is $\widetilde{P}_x$, by (2.18). Since I_q is positive definite, it follows that $\widetilde{P}_x \geqslant 0$ if and only if $F_x \geqslant 0$. On the other hand, since $\Delta \geqslant 0$, it follows from Lemma 1.6 that F_x is positive semidefinite if and only if

$$\mathrm{Ker}\,\Delta \subseteq \mathrm{Ker} \begin{bmatrix} M^* \\ D\mathbb{P}^{\frac{1}{2}}\mathbf{B}^* + \mathbf{e}E^* \end{bmatrix} \tag{2.24}$$

and the Schur complement of the block Δ in F_x is positive semidefinite:

$$\begin{bmatrix} I_q & x^* \\ x & \mathbf{e}\mathbf{e}^* + DD^* \end{bmatrix} - \begin{bmatrix} M^* \\ D\mathbb{P}^{\frac{1}{2}}\mathbf{B}^* + \mathbf{e}E^* \end{bmatrix} \Delta^{[-1]} \begin{bmatrix} M & E\mathbf{e}^* + \mathbf{B}\mathbb{P}^{\frac{1}{2}}D^* \end{bmatrix} \geqslant 0. \tag{2.25}$$

It follows from representations (2.17) of Δ that

$$\mathrm{Ker}\,\Delta = \mathrm{Ker}\,P^{\frac{1}{2}}G(z) \cap \mathrm{Ker}\,M^* \cap \mathrm{Ker}\,\mathbb{P}^{\frac{1}{2}}\mathbf{B}^* \cap \mathrm{Ker}\,E^*$$

and thus condition (2.24) is satisfied automatically. On the other hand, by (2.19) and (2.22), the matrix on the left-hand side of (2.25) coincides with K_x. Thus, taking into account Remark 2.1, we have

$$\widehat{P}_x \geqslant 0 \iff \widetilde{P}_x \geqslant 0 \iff K_x \geqslant 0,$$

which completes the proof of the first statement.

Since $\widetilde{P}_x$ is the Schur complement of the block I_q in the matrix F_x,

$$\mathrm{rank}\,F_x = q + \mathrm{rank}\,\widetilde{P}_x \quad \text{and} \quad \det F_x = \det I_q \cdot \det \widetilde{P}_x = \det \widetilde{P}_x.$$

Since K_x is the Schur complement of the block Δ in F_x,

$$\operatorname{rank} F_x = \operatorname{rank} \Delta + \operatorname{rank} K_x \quad \text{and} \quad \det F_x = \det \Delta \cdot \det K_x.$$

Thus,

$$\operatorname{rank} \widetilde{P}_x = \operatorname{rank} \Delta + \operatorname{rank} K_x - q \quad \text{and} \quad \det \widetilde{P}_x = \det \Delta \cdot \det K_x. \tag{2.26}$$

By (2.7), $\operatorname{rank} \widetilde{P}_x = \operatorname{rank} \widehat{P}_x$ and

$$\det \widetilde{P}_x = \det \widehat{P}_x \cdot |\det Q(z)|^2 = \det \widehat{P}_x \cdot |\det G(z)|^2 (1-|z|^2)^{k-n},$$

which together with relations (2.26) imply (2.20) and (2.21). □

Remark 2.4. The diagonal blocks

$$R_r = I_q - M^* \Delta^{[-1]} M \quad \text{and} \quad R_\ell = \begin{bmatrix} D & \mathbf{e} \end{bmatrix} \mathbf{P}_{\operatorname{Ker}[\mathbf{B}\mathbb{P}^{\frac{1}{2}} E]} \begin{bmatrix} D^* \\ \mathbf{e}^* \end{bmatrix} \tag{2.27}$$

in the matrix K_x are positive semidefinite.

Indeed, since by (2.17), $\Delta \geqslant MM^*$, it follows that $I_q - M^*\Delta^{[-1]}M \geqslant 0$. Positivity of R_ℓ is selfevident.

Now we can state the main result of this section.

Theorem 2.5. *Let conditions* (1.13) *be in force. Then x is a solution to Problem* 1.3 *if and only if it is of the form*

$$x = \begin{bmatrix} D & \mathbf{e} \end{bmatrix} \begin{bmatrix} \mathbb{P}^{\frac{1}{2}} \mathbf{B}^* \\ E^* \end{bmatrix} \Delta^{[-1]} M + R_\ell^{\frac{1}{2}} S R_r^{\frac{1}{2}} \tag{2.28}$$

for some matrix $S \in \mathbb{C}^{k\times q}$ with $\|S\| \leqslant 1$, where R_ℓ and R_r are the matrices given by (2.27).

Proof. By Lemma 2.3, the unique extension $\widehat{P}_x$ of P, subject to the extended Stein equation (1.7), is positive semidefinite if and only if the matrix K_x given by (2.19) is positive semidefinite. The diagonal blocks in K_x are positive semidefinite (by Remark 2.4) and thus, by the third statement in Lemma 1.6, K_x is positive semidefinite if and only if

$$x - \begin{bmatrix} D & \mathbf{e} \end{bmatrix} \begin{bmatrix} \mathbb{P}^{\frac{1}{2}} \mathbf{B}^* \\ E^* \end{bmatrix} \Delta^{[-1]} M = R_\ell^{\frac{1}{2}} S R_r^{\frac{1}{2}}$$

for some contractive matrix $S \in \mathbb{C}^{k\times q}$. The latter representation is equivalent to (2.28). □

Thus, the set

$$X = \left\{ x \in \mathbb{C}^{k\times q} : \widehat{P}_x \geqslant 0,\ \widehat{P}_x \text{ is subject to the Stein equation (1.7)} \right\} \tag{2.29}$$

of all solutions of Problem 1.2 is the matrix ball centered at

$$x_0 = \begin{bmatrix} D & y \end{bmatrix} \begin{bmatrix} \mathbb{P}^{\frac{1}{2}}\mathbf{B}^* \\ E^* \end{bmatrix} \varDelta^{[-1]} M \tag{2.30}$$

and with semiradii $R_\ell^{\frac{1}{2}}$ and $R_r^{\frac{1}{2}}$.

Note that the parameter S in the parametrization formula (2.28) is not independent: different contractive matrices S may lead via (2.28) to the same matrix x. However, if S varies over the set of contractive matrices such that $y^*Sx = 0$ for every $y \in \operatorname{Ker} R_\ell$ and $x \in \operatorname{Ker} R_r$, then formula (2.28) parameterizes the same matrix ball and different parameters lead to different solutions of Problem 1.2.

Corollary 2.6. *Problem* 1.2 *has a unique solution if and only if conditions* (1.13) *are in force and either*

$$\operatorname{rank} \varDelta = \operatorname{rank} P + q \quad \textit{or} \quad \operatorname{rank} \varDelta = \operatorname{rank} \begin{bmatrix} \mathbf{B}\mathbb{P}^{\frac{1}{2}} & E \\ D & \mathbf{e} \end{bmatrix}. \tag{2.31}$$

Proof. It follows from the representation (2.28) that the matrix ball X consists of one matrix if and only if at least one of the two semiradii R_ℓ and R_r is the zero matrix. By the Schur complement arguments,

$$\begin{aligned} \operatorname{rank} \begin{bmatrix} \varDelta & M \\ M^* & I_q \end{bmatrix} &= \operatorname{rank} \varDelta + \operatorname{rank} (I_q - M^* \varDelta^{[-1]} M) \\ &= \operatorname{rank} I_q + \operatorname{rank} (\varDelta - MM^*) \end{aligned}$$

and therefore,

$$\operatorname{rank} R_r = \operatorname{rank} (I_q - M^* \varDelta^{[-1]} M) = q + \operatorname{rank} (\varDelta - MM^*) - \operatorname{rank} \varDelta.$$

Since the matrix $G(z)$ is invertible, we get from (2.17)

$$\operatorname{rank} (\varDelta - MM^*) = \operatorname{rank} G(z)^* P G(z) = \operatorname{rank} P,$$

and therefore,

$$\operatorname{rank} R_r = \operatorname{rank} P + q - \operatorname{rank} \varDelta. \tag{2.32}$$

Thus, the condition $R_r = 0$ is equivalent to

$$\operatorname{rank} P + q - \operatorname{rank} \varDelta = 0,$$

that is, to the first condition in (2.31). On the other hand, it follows from (2.27) that the condition $R_\ell = 0$ is equivalent to

$$\begin{bmatrix} D & \mathbf{e} \end{bmatrix} \mathbf{P}_{\operatorname{Ker}[\mathbf{B}\mathbb{P}^{\frac{1}{2}} \, E]} = 0,$$

which, in turn, is equivalent to

$$\operatorname{rank} \begin{bmatrix} \mathbf{B}\mathbb{P}^{\frac{1}{2}} & E \\ D & \mathbf{e} \end{bmatrix} = \operatorname{rank} \begin{bmatrix} \mathbf{B}\mathbb{P}^{\frac{1}{2}} & E \end{bmatrix}.$$

The latter equality is equivalent to the second equality in (2.31), since

$$\operatorname{rank}\begin{bmatrix}\mathbf{B}\mathbb{P}^{\frac{1}{2}} & E\end{bmatrix} = \operatorname{rank}\begin{bmatrix}\mathbf{B}\mathbb{P}^{\frac{1}{2}} & E\end{bmatrix}\begin{bmatrix}\mathbb{P}^{\frac{1}{2}}\mathbf{B}^* \\ E^*\end{bmatrix} = \operatorname{rank}\varDelta. \qquad \square$$

3. Maximal and minimal rank extensions

According to (2.29), X stands for the set of all solutions of Problem 1.2. The question we address in this section is

Problem 3.1. Given $\widehat{T}_j$, $\widehat{E}$ and M, find the values

$$r_{\min} = \min_{x\in X} \operatorname{rank}\widehat{P}_x, \quad r_{\max} = \max_{x\in X} \operatorname{rank}\widehat{P}_x \tag{3.1}$$

and describe the sets

$$X_{\min} = \{x \in X : \operatorname{rank}\widehat{P}_x = r_{\min}\} \quad \text{and} \quad X_{\max} = \{x \in X : \operatorname{rank}\widehat{P}_x = r_{\max}\}.$$

Since for any positive semidefinite extension $\widehat{P} \in \mathbb{C}^{(n+k)\times(n+k)}$ of $P \in \mathbb{C}^{n\times n}$,

$$\operatorname{rank} P \leqslant \operatorname{rank}\widehat{P}_x \leqslant \operatorname{rank} P + k,$$

it follows immediately that

$$\operatorname{rank} P \leqslant r_{\min} \leqslant r_{\max} \leqslant \operatorname{rank} P + k.$$

However, these obvious bounds may not be attained under the assumption that $\widehat{P}$ is of a certain structure. The exact values of $r_{\max}$ and of $r_{\min}$ are given in the next theorem.

Theorem 3.2. *Let conditions* (1.13) *be in force and let R_ℓ and R_r be the matrices given by* (2.27). *Then*

$$r_{\min} = \begin{cases}\operatorname{rank} P & \text{if } \operatorname{rank} R_\ell \leqslant \operatorname{rank} R_r, \\ \operatorname{rank} P + \operatorname{rank} R_\ell - \operatorname{rank} R_r & \text{if } \operatorname{rank} R_\ell > \operatorname{rank} R_r,\end{cases} \tag{3.2}$$

and

$$r_{\max} = \operatorname{rank} P + \operatorname{rank} R_\ell. \tag{3.3}$$

The proof is based on the following lemma which is supplementary to Lemma 1.6 (to some extent) and is also well known.

Lemma 3.3. *Let the matrix $U = \begin{bmatrix} A & B^* \\ B & C\end{bmatrix}$ be positive semidefinite, where $A \in \mathbb{C}^{n\times n}$ and $C \in \mathbb{C}^{k\times k}$. Then*

$$\max\{\operatorname{rank} A, \operatorname{rank} C\} \leqslant \operatorname{rank} U \leqslant \operatorname{rank} A + \operatorname{rank} C. \tag{3.4}$$

Moreover,

1. $\operatorname{rank} U = \operatorname{rank} A + \operatorname{rank} C$ *if and only if B admits a representation*
$$B = C^{\frac{1}{2}} S A^{\frac{1}{2}}$$
for some strictly contractive matrix S.
2. *If* $\operatorname{rank} C \leqslant \operatorname{rank} A$, *then* $\operatorname{rank} U = \operatorname{rank} A$ *if and only if* $B = C^{\frac{1}{2}} S A^{\frac{1}{2}}$ *for some contractive matrix S such that*
$$\|\mathbf{P}_{\operatorname{Ran} A} S^* C g\| = \|Cg\| \quad \text{for every } g \in \mathbb{C}^k. \tag{3.5}$$
3. *If* $\operatorname{rank} C \geqslant \operatorname{rank} A$, *then* $\operatorname{rank} U = \operatorname{rank} C$ *if and only if* $B = C^{\frac{1}{2}} S A^{\frac{1}{2}}$ *for some contractive matrix S such that*
$$\|\mathbf{P}_{\operatorname{Ran} C} S A h\| = \|Ah\| \quad \text{for every } h \in \mathbb{C}^n. \tag{3.6}$$

Conditions (3.5) and (3.6) mean respectively that the operator
$$\widetilde{S} = \mathbf{P}_{\operatorname{Ran} C} S|_{\operatorname{Ran} A} : \operatorname{Ran} A \to \operatorname{Ran} C$$
is coisometric or isometric.

Proof. It follows from factorization formulas
$$\begin{aligned} U &= \begin{bmatrix} I_n & 0 \\ BA^{[-1]} & I_k \end{bmatrix} \begin{bmatrix} A & 0 \\ 0 & C - BA^{[-1]}B^* \end{bmatrix} \begin{bmatrix} I_n & A^{[-1]}B^* \\ 0 & I_k \end{bmatrix} \\ &= \begin{bmatrix} I_n & B^*C^{[-1]} \\ 0 & I_k \end{bmatrix} \begin{bmatrix} A - B^*C^{[-1]}B & 0 \\ 0 & C \end{bmatrix} \begin{bmatrix} I_n & 0 \\ C^{[-1]}B & I_k \end{bmatrix} \end{aligned}$$
that
$$\operatorname{rank} U = \operatorname{rank} A + \operatorname{rank}(C - BA^{[-1]}B^*) = \operatorname{rank} C + \operatorname{rank}(A - B^*C^{[-1]}B),$$
which imply inequalities (3.4).

By the third statement in Lemma 1.6, $B = C^{\frac{1}{2}} S A^{\frac{1}{2}}$ for some contractive matrix $S \in \mathbb{C}^{k\times n}$ and thus,
$$\begin{aligned} \operatorname{rank} U &= \operatorname{rank} A + \operatorname{rank}\big(C^{\frac{1}{2}}(I_k - SA^{\frac{1}{2}}A^{[-1]}A^{\frac{1}{2}}S^*)C^{\frac{1}{2}}\big) \\ &= \operatorname{rank} C + \operatorname{rank}\big(A^{\frac{1}{2}}(I_n - S^*C^{\frac{1}{2}}C^{[-1]}C^{\frac{1}{2}}S)A^{\frac{1}{2}}\big). \end{aligned}$$

Since, by the definition of the Moore–Penrose generalized inverse,
$$A^{\frac{1}{2}}A^{[-1]}A^{\frac{1}{2}} = \mathbf{P}_{\operatorname{Ran} A} \quad \text{and} \quad C^{\frac{1}{2}}C^{[-1]}C^{\frac{1}{2}} = \mathbf{P}_{\operatorname{Ran} C},$$
it follows that
$$\begin{aligned} \operatorname{rank} U &= \operatorname{rank} A + \operatorname{rank}\big(C^{\frac{1}{2}}(I_k - S\mathbf{P}_{\operatorname{Ran} A}S^*)C^{\frac{1}{2}}\big) \\ &= \operatorname{rank} C + \operatorname{rank}\big(A^{\frac{1}{2}}(I_n - S^*\mathbf{P}_{\operatorname{Ran} C}S)A^{\frac{1}{2}}\big), \end{aligned}$$

which imply immediately all the statements in the lemma. □

Proof of Theorem 3.2. Upon applying Lemma 3.3 to the positive semidefinite matrix

$$K_x = \begin{bmatrix} R_r & x^* - M^* \Delta^{[-1]} \begin{bmatrix} \mathbf{B}\mathbb{P}^{\frac{1}{2}} & E \end{bmatrix} \begin{bmatrix} D^* \\ \mathbf{e}^* \end{bmatrix} \\ x - \begin{bmatrix} D & \mathbf{e} \end{bmatrix} \begin{bmatrix} \mathbb{P}^{\frac{1}{2}}\mathbf{B}^* \\ E^* \end{bmatrix} \Delta^{[-1]} M & R_\ell \end{bmatrix}, \tag{3.7}$$

we get

$$\max\{\operatorname{rank} R_r, \operatorname{rank} R_\ell\} \leqslant \operatorname{rank} K_x \leqslant \operatorname{rank} R_r + \operatorname{rank} R_\ell. \tag{3.8}$$

Now we combine (2.20) and (3.8) to obtain

$$\max\{\operatorname{rank} R_r, \operatorname{rank} R_\ell\} + \operatorname{rank} \Delta - q \leqslant \operatorname{rank} \widehat{P}_x \leqslant \operatorname{rank} R_r + \operatorname{rank} R_\ell + \operatorname{rank} \Delta - q. \tag{3.9}$$

By (2.32),

$$\operatorname{rank} \Delta - q = \operatorname{rank} P - \operatorname{rank} R_r,$$

which being substituted into (3.9), leads to

$$\max\{\operatorname{rank} R_\ell - \operatorname{rank} R_r, 0\} + \operatorname{rank} P \leqslant \operatorname{rank} \widehat{P}_x \leqslant \operatorname{rank} P + \operatorname{rank} R_\ell,$$

which implies (3.2) and (3.3). □

Applying Statement 1 in Lemma 3.3 to the matrix K_x in (3.7), we arrive at

Theorem 3.4. *The set $X_{\max}$ of all matrices x leading to maximal rank positive semidefinite extensions $\widehat{P}_x$ is parametrized by the formula* (2.28), *where the parameter $S \in \mathbb{C}^{k\times q}$ varies on the set of all strictly contractive matrices.*

We leave it to the reader to apply Statements 2 and 3 in Lemma 3.3 to the matrix K_x to get a parametrization of the set $X_{\min}$.

4. Positive definite extensions

Using the preceding analysis, we can now treat Problem 1.3, which is a special case of a maximal rank positive semidefinite extension problem.

Theorem 4.1. *Problem* 1.3 *has a solution if and only if P satisfies the Stein identity* (1.3),

$$P > 0 \quad \textit{and} \quad R_\ell > 0, \tag{4.1}$$

where $R_\ell \in \mathbb{C}^{k\times k}$ *is the matrix given by* (2.27). *Moreover, if conditions* (1.3) *and* (4.1) *are in force, Problem* 1.3 *has infinitely many solutions* x, *which are parametrized by the formula*

$$x = \begin{bmatrix} D & \mathbf{e} \end{bmatrix} \begin{bmatrix} \mathbb{P}^{\frac{1}{2}}\mathbf{B}^* \\ E^* \end{bmatrix} \Delta^{-1} M + R_\ell^{\frac{1}{2}} S R_r^{\frac{1}{2}}, \tag{4.2}$$

where Δ *is the positive definite matrix defined as in* (2.17), *where*

$$R_r = I_q - M^* \Delta^{-1} M$$

and where S *is a free parameter running over the set of all* $k \times n$ *strictly contractive matrices.*

Proof. The necessity of (1.3) and of the first condition in (4.1) is clear. The necessity of the second condition in (4.1) can be established as follows: if $P > 0$, then for every positive definite $\widehat{P}_x$ subject to (1.7), it holds that

$$n + k = \operatorname{rank} \widehat{P}_x \leqslant \operatorname{rank} P + \operatorname{rank} R_\ell = n + \operatorname{rank} R_\ell. \tag{4.3}$$

Since R_ℓ is a $k \times k$ matrix, its rank does not exceed k and thus, it follows from (4.3) that $\operatorname{rank} R_\ell = k$. Since R_ℓ is clearly positive semidefinite, the third inequality in (4.1) follows.

If conditions (1.3) and (4.1) are in force, it follows from (2.17) that

$$\Delta \geqslant \frac{1}{1-|z|^2} G(z)^* P G(z) > 0$$

and thus, $\operatorname{rank} \Delta = n$. On account of (2.32),

$$\operatorname{rank} R_r = \operatorname{rank} P + q - \operatorname{rank} \Delta = q$$

and since R_r is a $q \times q$ matrix, it is positive definite. Furthermore, it follows from Theorem 3.2 that

$$r_{\max} = \operatorname{rank} P + \operatorname{rank} R_\ell = n + k$$

and thus, every maximal rank positive semidefinite extension $\widehat{P}_x$ is a positive definite extension of P and vice versa. Thus, the set of all solutions x of Problem 1.3 are parametrized by formula (4.2), which completes the proof. □

5. Maximal determinant extensions

In this section we consider another extremal problem related to Problem 1.2:

Problem 5.1. Maximize $\det \widehat{P}_x$ over the set of all solutions of Problem 1.2, i.e., find

$$\delta = \max_{x\in X} \det \widehat{P}_x$$

and a matrix x_0 for which $\det \widehat{P}_x = \delta$.

We refer to [14,16] where this problem was considered from an interpolation point of view (connections of structured positive semidefinite extension problems with interpolation will be discussed in Section 7).

In the case when at least one inequality in (4.1) fails, the maximum determinant extension problem becomes trivial: any solution x of Problem 1.2 leads to a singular $\widehat{P}_x$ and thus, any positive semidefinite extension $\widehat{P}_x$ has the possibly maximal determinant, which is zero. The complementary case is covered by the following:

Theorem 5.2. *Let conditions* (1.3) *and* (4.1) *be in force*. *Then*

$$\delta := \max_{x\in X} \det \widehat{P}_x = (1-|z|^2)^{-k} \det P \cdot \det R_\ell \tag{5.1}$$

and moreover, $\det \widehat{P}_x = \delta$ *if and only if*

$$x = \begin{bmatrix} D & \mathbf{e} \end{bmatrix} \begin{bmatrix} \mathbb{P}^{\frac{1}{2}}\mathbf{B}^* \\ E^* \end{bmatrix} \Delta^{-1} M. \tag{5.2}$$

Proof. The proof is based on relation (2.21) in Lemma 2.3 and the following simple and well known result: *If the matrix* $U = \begin{bmatrix} A & B^* \\ B & C \end{bmatrix}$ *is positive definite, then*

$$\det U = \det A \cdot \det(C - BA^{-1}B^*) \leqslant \det A \cdot \det C$$

with equality if and only if $B = 0$.

We apply this result to the matrix K_x in (3.7) (note that in the present context, i.e., under assumption that $P > 0$, the matrix Δ defined by (2.17) is positive definite; thus we use Δ^{-1} in (3.7), rather than $\Delta^{[-1]}$) to conclude that

$$\det K_x \leqslant \det R_\ell \cdot \det R_r, \tag{5.3}$$

with equality if and only if x is of the form (5.2). Making use of (2.21) and taking into account (5.3), we arrive at

$$\begin{aligned} \det \widehat{P}_x &= (1-|z|^2)^{n-k} \frac{\det \Delta \cdot \det K_x}{|\det G(z)|^2} \\ &\leqslant (1-|z|^2)^{n-k} \frac{\det \Delta \cdot \det R_\ell \cdot \det R_r}{|\det G(z)|^2} \end{aligned} \tag{5.4}$$

with equality if and only if x is of the form (5.2). To complete the proof, it remains to note that in view of (2.27) and (2.17),

$$\begin{aligned} \det \Delta \cdot \det R_r &= \det \Delta \cdot \det(I_q - M^*\Delta^{-1}M) \\ &= \det \Delta \cdot \det(I_q - \Delta^{-1}MM^*) \\ &= \det(\Delta - MM^*) = \det\left(\frac{G(z)^*PG(z)}{1-|z|^2}\right) \\ &= (1-|z|^2)^{-n} |\det G(z)|^2 \cdot \det P, \end{aligned}$$

which upon being substituted into (5.4), leads to the desired conclusion. □

We have already mentioned that Problem 5.1 does not make much sense if conditions (4.1) are not in force (although formula (5.1) for δ is true in any case). In conclusion we suggest two different modifications of Problem 5.1, each of which reduces to Problem 5.1 when conditions (4.1) are in force, and yet remains meaningful when these conditions are not met.

Given a positive semidefinite matrix $A \in \mathbb{C}^{n\times n}$, let $\mathbf{D}_\ell[A]$ denote the sum of all its principal minors of order $\ell \leqslant n$. It is clear that if A is positive definite, then $\mathbf{D}_n[A] = \det A$. Moreover, if rank $P = r$, then $\mathbf{D}_r[A]$ is equal to the product of all the positive eigenvalues of A.

Remark 5.3. Note also that if A is positive semidefinite, then $\mathbf{D}_\ell[A] = 0$ if and only if $\ell >$ rank A.

Problem 5.4. Maximize $\mathbf{D}_{r+k}[\widehat{P_x}]$ over the set of all solutions of Problem 1.2, where $r =$ rank P.

The idea of considering $\mathbf{D}_\ell[P]$ (with an appropriate ℓ) instead of det P goes back to Inouye [18] who has used it to define an entropy functional for regular random processes with degenerate rank. In the context of structured positive semidefinite extensions, this idea was realized in [9, Section 12], where Problem 5.4 was considered for the case when $d = 1$.

By (3.3), the possibly maximal rank of $\widehat{P_x}$ equals rank $P +$ rank R_ℓ, and so it follows, by Remark 5.3, that

$$\delta := \max_{x\in X} \mathbf{D}_{r+k}[\widehat{P_x}]$$

is positive if and only if rank $R_\ell = k$, that is, if and only if $R_\ell > 0$. Otherwise, $\delta = 0$ and for every $x \in X$, it holds that $\mathbf{D}_{r+k}[\widehat{P_x}] = 0$. Thus, Problem 5.4 is meaningful for possibly singular P, but only under the assumption that R_ℓ is positive definite.

To get rid of this halved situation we arrive at the following:

Problem 5.5. Maximize $\mathbf{D}_{r_{\max}}[\widehat{P_x}]$ over the set of all solutions of Problem 1.2, where $r_{\max}$ is the integer defined in (3.3).

In this case, the number

$$\delta := \max_{x\in X} \mathbf{D}_{r_{\max}}[\widehat{P_x}]$$

is clearly positive and the problem makes sense for any initial data. It is also clear that the nontrivial case of Problem 5.4 (when $R_\ell > 0$) is a particular case of Problem 5.5.

We do not know any reasonable analogue of relation (2.21) for variants $\mathbf{D}_\ell$'s instead of determinants; apparently the approach used above to solve Problem 5.1 cannot be applied to Problems 5.4 and 5.5. For $d = 1$, Problem 5.4 was treated in [9] using heavily interpolation theory for analytic contractive valued functions on the unit disk (Schur functions). As we have already remarked in Section 1, the existing results in multivariable interpolation theory do not allow us to apply that approach in full generality.

6. Positive definite kernel extensions

In this section we describe all the solutions of Problem 1.7 for the case when P is positive definite. Then, using "structured" regularization in the spirit of [19], we shall show that if P is positive semidefinite, Problem 1.7 has a solution.

Upon substituting (1.9), (1.15) and (1.16) into (1.17) and comparing the corresponding blocks, we come to the equalities

$$\beta - \sum_{j=1}^{d} z_j \beta T_j^* = \mathbf{e}(z)E^* - x(z)M^*,$$
$$\gamma - \sum_{j=1}^{d} z_j \bar{w}_j^* \gamma = \mathbf{e}(z)\mathbf{e}(w)^* - x(z)x(w)^*,$$

which imply (note that in the present context, β and γ turn out to be functions)

$$\beta(z) = (\mathbf{e}(z)E^* - x(z)M^*)G(z)^{-1},$$
$$\gamma(z, w) = \frac{\mathbf{e}(z)\mathbf{e}(w)^* - x(z)x(w)^*}{1 - \langle z, w\rangle},$$

where $G(z)$ is the function defined in (1.6) and where

$$\langle z, w\rangle = \sum_{j=1}^{d} z_j \bar{w}_j$$

is the standard inner product of $\mathbb{C}^d$. Thus, the unique extension $\widehat{P}_x(z, w)$ of P, subject to the Stein identity (1.17), is of the form

$$\widehat{P}_x(z, w) = \begin{bmatrix} P & G(w)^{-*}\left(E\mathbf{e}(w)^* - Mx(w)^*\right) \\ \left(\mathbf{e}(z)E^* - x(z)M^*\right)G(z)^{-1} & \frac{\mathbf{e}(z)\mathbf{e}(w)^* - x(z)x(w)^*}{1-\langle z,w\rangle} \end{bmatrix} \tag{6.1}$$

and Problem 1.7 can be reformulated as follows (for convenience, we include the necessary conditions (1.13) into the formulation of the problem).

Problem 6.1. Given matrices T_j, E, M and $P \geqslant 0$ subject to the Stein identity (1.3), find all $\mathbb{C}^{k\times q}$ valued functions x such that the kernel $\widehat{P}_x(z, w)$ of the form (6.1) is positive definite on $\mathbb{B}^d \times \mathbb{B}^d$.

Note an important particular case of the latter problem, corresponding to the choice of $k = p$, $\mathbf{e}(z) \equiv I_p$ and $x(z) = S(z)$.

Problem 6.2. Given matrices T_j, E, M and $P \geqslant 0$ subject to the Stein identity (1.3), find all $\mathbb{C}^{k\times q}$-valued functions x such that the following kernel is positive definite on $\mathbb{B}^d \times \mathbb{B}^d$:

$$\widehat{P}_S(z, w) = \begin{bmatrix} P & G(w)^{-*}\,(E - MS(w)^*) \\ (E^* - S(z)M^*)\,G(z)^{-1} & \frac{I_p - S(z)S(w)^*}{1-\langle z, w\rangle} \end{bmatrix} \succeq 0. \tag{6.2}$$

For every solution S of Problem 6.2, the kernel

$$K_S(z, w) = \frac{I_p - S(z)S(w)^*}{1 - \langle z, w\rangle} \tag{6.3}$$

is positive definite on $\mathbb{B}^d \times \mathbb{B}^d$. We shall denote by $\mathscr{S}_d^{p\times q}$ the set of all $\mathbb{C}^{p\times q}$-valued functions S defined on $\mathbb{B}^d$ and such that the kernel K_S is positive definite on $\mathbb{B}^d \times \mathbb{B}^d$; positivity of the kernel K_S on $\mathbb{B}^d \times \mathbb{B}^d$ implies that S is necessarily analytic on $\mathbb{B}^d$. Functions of the class $\mathscr{S}_d^{p\times q}$ and their operator-valued analogues have been studied recently quite intensively (see [1,6,17] and references there). Turning back to Problem 6.2, note that positivity of the "whole" kernel $\widehat{P}_S(z, w)$ in (6.2) imposes certain restriction on $S \in \mathscr{S}_d^{p\times q}$, which will be clarified (to some extent) below.

Problem 6.2 is of particular interest for us, since it turns out to be equivalent to (a more general) Problem 6.1 in the following sense:

Theorem 6.3. *Let P be a positive semidefinite solution of the Stein equation* (1.3). *Then the kernel $\widehat{P}_x(z, w)$ of the form* (6.1) *is positive definite on $\mathbb{B}^d \times \mathbb{B}^d$ if and only if x is of the form*

$$x(z) = \mathbf{e}(z)S(z) \tag{6.4}$$

for some $\mathbb{C}^{p\times q}$-valued function S satisfying (6.2).

In other words, x is a solution of Problem 6.1 if and only if it is of the form (6.4) for some solution S of Problem 6.2.

Proof. The sufficiency part is obvious: let x be of the form (6.4) and let (6.2) be in force. Due to (6.4), it holds that

$$\widehat{P}_x(z, w) = \begin{bmatrix} I_n & 0 \\ 0 & \mathbf{e}(z) \end{bmatrix} \widehat{P}_S(z, w) \begin{bmatrix} I_n & 0 \\ 0 & \mathbf{e}(w)^* \end{bmatrix}, \tag{6.5}$$

which forces $\widehat{P}_x(z, w) \succeq 0$, by (6.2).

The necessity part is less trivial. The proof is partially based on the following result. □

Theorem 6.4. *Let* $\mathbf{e}$ *and* x *be two matrix-valued functions, defined on* $\mathbb{B}^d$. *Then the kernel*

$$\frac{\mathbf{e}(z)\mathbf{e}(w)^* - x(z)x(w)^*}{1 - \langle z, w\rangle} \tag{6.6}$$

is positive on $\mathbb{B}^d \times \mathbb{B}^d$ *if and only if* x *admits a representation* (6.4) *with some matrix-valued function* S (*of an appropriate size*) *of the class* $\mathscr{S}_d$ (*i.e., such that the kernel* K_S *in* (6.3) *is positive definite on* $\mathbb{B}^d \times \mathbb{B}^d$).

As in Theorem 6.3, only the necessity part here is nontrivial; we refer to [5, Section 6.1] for the proof of this result (where it is presented in a more general operator-valued bitangential setting). Note also that in the one-variable formulation ($d = 1$), Theorem 6.4 appeared first in [23]; the complete proof was given in [24] and reproduced later in [10] (since the source [24] is hardly reachable). Under the assumption that $\mathbf{e}$ and x are analytic, the one-variable result is known as Leech's theorem and becomes an easy but elegant consequence of the commutant lifting theorem [31, p. 107].

Positivity of the kernel $\widehat{P}_x(z, w)$ of the form (6.1) contains, besides positivity of the kernel (6.6) some more information about the function x. In fact, the necessity part in Theorem 6.3 asserts that this additional information is contained completely in the factor S from the representation (6.4).

Making use of Theorem 6.4, one can prove easily the necessity part in Theorem 6.3 under the additional (and actually, quite restrictive) assumption that

$$\operatorname{rank} \mathbf{e}(z) = p \quad (z \in \mathbb{B}^d).$$

Indeed, assuming that the kernel $\widehat{P}_x(z, w)$ is positive definite (and therefore, that the kernel (6.6) is positive definite), we conclude, by Theorem 6.4 that x admits a factorization (6.4) for some function $S \in \mathscr{S}_d^{p\times q}$. Then relation (6.5) holds and (6.1) follows. However, if $\mathbf{e}(z)$ is not invertible from the left, positivity of $\widehat{P}_S(z, w)$ does not follow directly from (6.5). We shall complete the proof in Section 7.

The next remark is a simple "kernel" analogue of Remark 1.5.

Remark 6.5. Let $P > 0$. Then the kernel

$$\widehat{P}_x(z, w) = \begin{bmatrix} P & \beta(w)^* \\ \beta(z) & \gamma(z, w) \end{bmatrix}$$

is positive definite on $\Omega \times \Omega$ if and only if the kernel $\gamma(z, w) - \beta(z)P^{-1}\beta(w)^*$ is positive definite on $\Omega \times \Omega$.

The assertion follows from the factorization formula

$$\widehat{P}_x(z,w)=\begin{bmatrix} I & 0\\ \beta(z)P^{-1} & I\end{bmatrix}\begin{bmatrix} P & 0\\ 0 & \gamma(z,w)-\beta(z)P^{-1}\beta(w)^*\end{bmatrix}\begin{bmatrix} I & P^{-1}\beta(w)^*\\ 0 & I\end{bmatrix}.$$

In the case when $P>0$, we use Remark 6.5 to conclude that positivity of the kernel (6.1) is equivalent to

$$\frac{\mathbf{e}(z)\mathbf{e}(w)^*-x(z)x(w)^*}{1-\langle z,w\rangle} \\ -(\mathbf{e}(z)E^*-x(z)M^*)G(z)^{-1}P^{-1}G(w)^{-*}(E\mathbf{e}(w)^*-Mx(w)^*)\succeq 0,$$

which in turn, can be written as

$$\begin{bmatrix}\mathbf{e}(z) & -x(z)\end{bmatrix}\left\{\frac{J}{1-\langle z,w\rangle} - \begin{bmatrix}E^*\\ M^*\end{bmatrix}G(z)^{-1}P^{-1}G(w)^{-*}\begin{bmatrix}E & M\end{bmatrix}\right\}\begin{bmatrix}\mathbf{e}(w)^*\\ -x(w)^*\end{bmatrix}\succeq 0, \tag{6.7}$$

where

$$J=\begin{bmatrix} I_p & 0\\ 0 & -I_q\end{bmatrix}. \tag{6.8}$$

It turns out that the $\mathbb{C}^{(p+q)\times(nd+p+q)}$-valued function

$$\Theta(z)=\begin{bmatrix}0 & I_{p+q}\end{bmatrix}+\begin{bmatrix}E^*\\ M^*\end{bmatrix}G(z)^{-1}P^{-1}\begin{bmatrix}(Z(z)-\mathbf{T})\mathbb{P}^{\frac{1}{2}} & -E & M\end{bmatrix} \tag{6.9}$$

(which clearly is analytic in $\mathbb{B}^d$) satisfies the following identity

$$\frac{J-\Theta(z)\mathbf{J}\Theta(w)^*}{1-\langle z,w\rangle}=\begin{bmatrix}E^*\\ M^*\end{bmatrix}G(z)^{-1}P^{-1}G(w)^{-*}\begin{bmatrix}E & M\end{bmatrix}\quad (z,w\in\mathbb{B}^d), \tag{6.10}$$

where

$$\mathbf{J}=\begin{bmatrix} I_{nd} & 0\\ 0 & J\end{bmatrix}=\begin{bmatrix} I_{nd+p} & 0\\ 0 & -I_q\end{bmatrix}. \tag{6.11}$$

The proof of (6.10) (based on the identity (1.3) only) is straightforward and can be found in [8, p. 1381].

Taking advantage of (6.10), we rewrite the last inequality (6.7) as

$$\begin{bmatrix}\mathbf{e}(z) & -x(z)\end{bmatrix}\frac{\Theta(z)\mathbf{J}\Theta(w)^*}{1-\langle z,w\rangle}\begin{bmatrix}\mathbf{e}(w)^*\\ -x(w)^*\end{bmatrix}\succeq 0\quad (z,w\in\mathbb{B}^d). \tag{6.12}$$

Theorem 6.6. *Let P be positive definite and let*

$$\Theta=\begin{bmatrix}\Theta_{11} & \Theta_{12}\\ \Theta_{21} & \Theta_{22}\end{bmatrix}:\begin{bmatrix}\mathbb{C}^{nd+p}\\ \mathbb{C}^q\end{bmatrix}\to\begin{bmatrix}\mathbb{C}^p\\ \mathbb{C}^q\end{bmatrix} \tag{6.13}$$

be the partition of the function Θ given by (6.9) *into four blocks of the indicated sizes. Then the set of all solutions x of Problem* 1.7 *is parametrized by the linear fractional transformation*

$$x(z) = \mathbf{e}(z)\,(\Theta_{11}(z)\mathscr{E}(z) + \Theta_{12}(z))\,(\Theta_{21}(z)\mathscr{E}(z) + \Theta_{22}(z))^{-1}\,, \tag{6.14}$$

when the parameter $\mathscr{E}$ varies on the set $\mathscr{S}_d^{(nd+p)\times q}$.

Proof. It follows from (6.10), (6.8), (6.11) and (6.13) that

$$-I_q - \Theta_{21}(z)\Theta_{21}(z)^* + \Theta_{22}(z)\Theta_{22}(z)^* \geqslant 0 \quad (z \in \mathbb{B}^d).$$

Therefore, $\Theta_{22}(z)$ is invertible at every point $z \in \mathbb{B}^d$ and $\|\Theta_{22}(z)^{-1}\Theta_{21}(z)\| < 1$. Then the function

$$\Theta_{21}(z)\mathscr{E}(z) + \Theta_{22}(z) = \Theta_{22}(z)(\Theta_{22}(z)^{-1}\Theta_{21}(z)\mathscr{E}(z) + I_q)$$

is invertible in $\mathbb{B}^d$ for every $\mathscr{E} \in \mathscr{S}^{(nd+p)\times q}$, which means that the transformation (6.14) is well defined on the set $\mathscr{S}_d^{(nd+p)\times q}$.

According to the preceding analysis, x is a solution of Problem 1.7 if and only if it satisfies the inequality (6.12). Setting

$$\begin{bmatrix} u(z) & -v(z) \end{bmatrix} = \begin{bmatrix} \mathbf{e}(z) & -x(z) \end{bmatrix} \Theta(z), \tag{6.15}$$

where u and v are, respectively, $\mathbb{C}^{p\times(nd+p)}$- and $\mathbb{C}^{p\times q}$-valued, one can rewrite (6.12) as

$$\frac{u(z)u(w)^* - v(z)v(w)^*}{1 - \langle z, w\rangle} \succeq 0 \quad (z, w \in \mathbb{B}^d),$$

which is equivalent (by Theorem 6.4) to the existence of a function $\mathscr{E} \in \mathscr{S}_d^{(nd+p)\times q}$ such that

$$u(z)\mathscr{E}(z) = v(z) \quad (z \in \mathbb{B}^d).$$

By (6.15), we conclude that x is a solution of Problem 1.7 if and only if

$$\begin{bmatrix} \mathbf{e}(z) & -x(z) \end{bmatrix} \Theta(z) = u(z) \begin{bmatrix} I_{nd+p} & -\mathscr{E}(z) \end{bmatrix}$$

for some function u defined on $\mathbb{B}^d$ and a function $\mathscr{E} \in \mathscr{S}_d^{(nd+p)\times q}$. The latter is equivalent to

$$\begin{bmatrix} \mathbf{e}(z) & -x(z) \end{bmatrix} \Theta(z) \begin{bmatrix} \mathscr{E}(z) \\ I_q \end{bmatrix} = 0,$$

which, being rewritten as

$$\mathbf{e}(z)\,(\Theta_{11}(z)\mathscr{E}(z) + \Theta_{12}(z)) - x(z)\,(\Theta_{21}(z)\mathscr{E}(z) + \Theta_{22}(z)) = 0$$

is evidently equivalent to (6.14). $\square$

As a consequence of the last theorem we get that under the assumption $P > 0$, Problem 1.7 has infinitely many solutions. Using a suitable regularization, we shall show in the next theorem that

Theorem 6.7. *Problem* 6.1 *always has a solution.*

Proof. Let $\{\varepsilon_i\}$ be any decreasing positive sequence tending to zero and let

$$E_{\varepsilon_i} = \begin{bmatrix} E & \varepsilon_i I_n \end{bmatrix}, \quad M_{\varepsilon_i} = \begin{bmatrix} M & \varepsilon_i \mathbf{T} \end{bmatrix}, \quad P_{\varepsilon_i} = P + \varepsilon_i^2 I_n. \tag{6.16}$$

Furthermore, let us introduce the extended matrices $\widehat{E}_{\varepsilon_i}(z)$ and $\widehat{M}_{\varepsilon_i}(z)$ by

$$\widetilde{E}_{\varepsilon_i}(z) = \begin{bmatrix} E & \varepsilon_i I_n \\ \mathbf{e}(z) & 0 \end{bmatrix}, \quad \widetilde{M}_{\varepsilon_i}(z) = \begin{bmatrix} M & \varepsilon_i \mathbf{T} \\ x_{1,\varepsilon_i}(z) & x_{2,\varepsilon_i}(z) \end{bmatrix}.$$

Then the matrix P_{ε_i} is positive definite and satisfies the Stein identity

$$P_{\varepsilon_i} - \sum_{j=1}^{d} T_j P_{\varepsilon_i} T_j^* = E_{\varepsilon_i} E_{\varepsilon_i}^* - M_{\varepsilon_i} M_{\varepsilon_i}^*. \tag{6.17}$$

Then, by Theorem 6.6, for every i, there exists a function

$$x_{\varepsilon_i}(z) = \begin{bmatrix} x_{1,\varepsilon_i}(z) & x_{2,\varepsilon_i}(z) \end{bmatrix} \tag{6.18}$$

such that the unique extension $\widehat{P}_{\varepsilon_i,x}(z,w)$ of P_{ε_i}, subject to extended Stein identity

$$\widehat{P} - \sum_{j=1}^{d} \widehat{T}_j(z)\widehat{P}\,\widehat{T}_j(w)^* = \widehat{E}_{\varepsilon_i}(z)\widehat{E}_{\varepsilon_i}(w)^* - \widehat{M}_{\varepsilon_i}(z)\widehat{M}_{\varepsilon_i}(w)^* \tag{6.19}$$

is a positive kernel on $\mathbb{B}^d$. The explicit formula for $\widehat{P}_{\varepsilon_i,x}(z,w)$ is derived from (6.19) and is similar to (6.1):

$$\widehat{P}_{\varepsilon_i,x}(z,w) = \begin{bmatrix} P_{\varepsilon_i} & W_{\varepsilon_i}(w)^* \\ W_{\varepsilon_i}(z) & \frac{\mathbf{e}(z)\mathbf{e}(w)^* - x_{\varepsilon_i}(z)x_{\varepsilon_i}(w)^*}{1-\langle z,w\rangle} \end{bmatrix} \succeq 0, \tag{6.20}$$

where

$$W_{\varepsilon_i}(z) = \left(\begin{bmatrix} \mathbf{e}(z) & 0 \end{bmatrix} E_{\varepsilon_i}^* - x_{\varepsilon_i}(z) M_{\varepsilon_i}^*\right) G(z)^{-1}. \tag{6.21}$$

It follows from (6.19) that, in particular,

$$\frac{\mathbf{e}(z)\mathbf{e}(w)^* - x_{\varepsilon_i}(z)x_{\varepsilon_i}(w)^*}{1-\langle z,w\rangle} \succeq 0 \quad (z,w \in \mathbb{B}^d)$$

and then, by Theorem 6.4, there exists a function $S_{\varepsilon_i} \in \mathscr{S}_d^{p\times(q+nd)}$ such that

$$x_{\varepsilon_i}(z) = \mathbf{e}(z) S_{\varepsilon_i}(z). \tag{6.22}$$

Since the functions S_{ε_i}'s are analytic and contractive valued on $\mathbb{B}^d$, there exists (by Montel's theorem) a subsequence of $\{\varepsilon_i\}$ (for which we shall keep the same notation) such that $\{S_{\varepsilon_i}\}$ converges to an analytic function $S(z)$ uniformly on compact subsets of $\mathbb{B}^d$. Since $S_{\varepsilon_i} \in \mathscr{S}_d^{p\times(q+nd)}$, the kernels $K_{S_i}(z,w) = \frac{I_p - S_{\varepsilon_i}(z)S_{\varepsilon_i}(w)^*}{1-\langle z,w\rangle}$ are positive definite on $\mathbb{B}^d$. By approximation arguments, the limit kernel $K_S(z,w)$ is positive definite on $\mathbb{B}^d \times \mathbb{B}^d$ and thus, the limit function S is of the class $\mathscr{S}_d^{p\times(q+nd)}$. Passing to limits in (6.22) we come to the function

$$\hat{x}(z) = \lim_{i\to\infty} x_{\varepsilon_i}(z) = \mathbf{e}(z)S(z). \tag{6.23}$$

Let

$$\hat{x}(z) = \begin{bmatrix}\hat{x}_1(z) & \hat{x}_2(z)\end{bmatrix} \tag{6.24}$$

be the partitioning of $\hat{x}$ conformal with (6.18). Then it follows from (6.21) that

$$\lim_{i\to\infty} W_{\varepsilon_i}(z) = (\mathbf{e}(z)E^* - \hat{x}_1(z)M^*)G(z)^{-1}.$$

Now we pass to limits in (6.20) (as $i \to \infty$) to get the positive kernel

$$\widehat{P}_{\hat{x}}(z,w) = \begin{bmatrix} P & G(w)^{-*}(E\mathbf{e}(w)^* - M\hat{x}_1(w)^*) \\ (\mathbf{e}(z)E^* - \hat{x}_1(z)M^*)G(z)^{-1} & \frac{\mathbf{e}(z)\mathbf{e}(w)^* - \hat{x}(z)\hat{x}(w)^*}{1-\langle z,w\rangle} \end{bmatrix} \succeq 0.$$

Adding to the latter kernel the positive kernel $\begin{bmatrix} 0 & 0 \\ 0 & \hat{x}_2(z)\hat{x}_2(w)^* \end{bmatrix}$ and taking into account that

$$\hat{x}(z)\hat{x}(w)^* = \hat{x}_1(z)\hat{x}_1(w)^* + \hat{x}_2(z)\hat{x}_2(w)^*,$$

due to (6.24), we get

$$\widehat{P}_{\hat{x}_1}(z,w) = \begin{bmatrix} P & G(w)^{-*}(E\mathbf{e}(w)^* - M\hat{x}_1(w)^*) \\ (\mathbf{e}(z)E^* - \hat{x}_1(z)M^*)G(z)^{-1} & \frac{\mathbf{e}(z)\mathbf{e}(w)^* - \hat{x}_1(z)\hat{x}_1(w)^*}{1-\langle z,w\rangle} \end{bmatrix} \succeq 0.$$

The latter kernel is a unique extension of P, subject to extended Stein equation

$$\widehat{P} - \sum_{j=1}^{d} \widehat{T}_j(z)\widehat{P}\,\widehat{T}_j(w)^* = \begin{bmatrix} E \\ \mathbf{e}(z) \end{bmatrix}\begin{bmatrix} E^* & \mathbf{e}(w)^* \end{bmatrix} - \begin{bmatrix} E \\ \hat{x}_1(z) \end{bmatrix}\begin{bmatrix} E^* & \hat{x}_1(w)^* \end{bmatrix},$$

which means that $\hat{x}_1$ is a solution of Problem 1.7. $\square$

Note that regularization (6.16) is quite special: to apply Theorem 6.6 (i.e., the nonsingular case) we had to regularize P to make its regularization P_ε not only positive definite, but also satisfy certain Stein identity. To our best knowledge such structured regularization was first suggested in [19] (see also [20]).

We mention another consequence of Theorem 6.6. In the case when $k = p$, $\mathbf{e}(z) \equiv I_p$ and $x(z) = S(z)$, Theorem 6.6 reads:

Theorem 6.8. *Let P be positive definite solution of the Stein equation* (1.3) *and let Θ be the function defined in* (6.9) *and partitioned into four blocks as in* (6.13).

Then the set of all solutions S of Problem 6.2 *is parametrized by the linear fractional transformation*

$$S(z) = (\Theta_{11}(z)\mathscr{E}(z) + \Theta_{12}(z))\,(\Theta_{21}(z)\mathscr{E}(z) + \Theta_{22}(z))^{-1}\,, \tag{6.25}$$

when the parameter $\mathscr{E}$ *varies on the set* $\mathscr{S}_d^{(nd+p)\times q}$.

7. Positive kernel extensions and interpolation

We start this section with the proof of the necessity part in Theorem 6.3.

Proof of Theorem 6.3 (*necessity part*). Let $x(z)$ be such that the kernel $\widehat{P}_x(z,w)$ of the form (6.1) is positive definite. We consider separately two cases.

Case 1: $P > 0$. In this case one can define the function Θ by formula (6.9) and conclude, by Theorem 6.6, that x admits a representation (6.14):

$$x(z) = \mathbf{e}(z)\,(\Theta_{11}(z)\mathscr{E}(z) + \Theta_{12}(z))\,(\Theta_{21}(z)\mathscr{E}(z) + \Theta_{22}(z))^{-1}\,,$$

with some function $\mathscr{E} \in \mathscr{S}_d^{(nd+p)\times q}$. Thus,

$$x(z) = \mathbf{e}(z)S(z),$$

where

$$S(z) := (\Theta_{11}(z)\mathscr{E}(z) + \Theta_{12}(z))\,(\Theta_{21}(z)\mathscr{E}(z) + \Theta_{22}(z))^{-1}\,. \tag{7.1}$$

But by Theorem 6.8, the function S of the form (7.1) is a solution of Problem 6.2, i.e., it satisfies (6.2).

Case 2: $P \geqslant 0$. In this case we use regularization arguments, similar to those in the proof of Theorem 6.7 (note that in the contrast to Theorem 6.7, now we start with certain $x(z)$ such that the kernel $\widehat{P}_x(z,w)$ is positive definite). Let $\{\varepsilon_i\}$ be any decreasing positive sequence tending to zero and let (as in (6.16))

$$E_{\varepsilon_i} = \begin{bmatrix} E & \varepsilon_i I_n \end{bmatrix}, \quad M_{\varepsilon_i} = \begin{bmatrix} M & \varepsilon_i \mathbf{T} \end{bmatrix}, \quad P_{\varepsilon_i} = P + \varepsilon_i^2 I_n. \tag{7.2}$$

Furthermore, we let

$$\hat{\mathbf{e}}(z) = \begin{bmatrix} \mathbf{e}(z) & 0 \end{bmatrix}, \quad \hat{x}(z) = \begin{bmatrix} x(z) & 0 \end{bmatrix} \tag{7.3}$$

and

$$\widehat{E}_{\varepsilon_i}(z) = \begin{bmatrix} E_{\varepsilon_i} \\ \hat{\mathbf{e}}(z) \end{bmatrix}, \quad \widehat{M}_{\varepsilon_i}(z) = \begin{bmatrix} M_{\varepsilon_i} \\ \hat{x}(z) \end{bmatrix}.$$

It is easily seen that a unique extension $\widehat{P}_{\hat{x},\varepsilon_i}$ of P_{ε_i}, subject to extended Stein equation (6.19), takes the form

$$\widehat{P}_{\hat{x},\varepsilon_i}(z,w) = \begin{bmatrix} P_{\varepsilon_i} & G(w)^{-*}\left(E_{\varepsilon_i}\hat{\mathbf{e}}(w)^* - M_{\varepsilon_i}\hat{x}(w)^*\right) \\ \left(\hat{\mathbf{e}}(z)E_{\varepsilon_i}^* - \hat{x}(z)M_{\varepsilon_i}^*\right)G(z)^{-1} & \frac{\hat{\mathbf{e}}(z)\hat{\mathbf{e}}(w)^* - \hat{x}(z)\hat{x}(w)^*}{1-\langle z,w\rangle} \end{bmatrix}, \tag{7.4}$$

which is the same (due to (7.2) and (7.3)) as

$$\widehat{P}_{\hat{x},\varepsilon_i}(z,w)=\begin{bmatrix} P_{\varepsilon_i} & G(w)^{-*}\left(E\mathbf{e}(w)^*-Mx(w)^*\right) \\ \left(\mathbf{e}(z)E^*-x(z)M^*\right)G(z)^{-1} & \frac{\mathbf{e}(z)\mathbf{e}(w)^*-x(z)x(w)^*}{1-\langle z,w\rangle}\end{bmatrix}.$$

Comparing the last formula with (6.1) we see that

$$\widehat{P}_{\hat{x},\varepsilon_i}(z,w)=\widehat{P}_x(z,w)+\begin{bmatrix}\varepsilon_i^2 I_n & 0\\ 0 & 0\end{bmatrix}$$

and thus, the assumption $\widehat{P}_x(z,w)\succeq 0$ implies that $\widehat{P}_{\hat{x},\varepsilon_i}(z,w)\succeq 0$. Since P_{ε_i} is positive definite and satisfies the Stein identity (6.17), we can apply Case 1 to the kernel (7.4) to conclude that

$$\hat{x}(z)=\hat{\mathbf{e}}(z)S_{\varepsilon_i}(z)$$

or equivalently, that

$$\begin{bmatrix}x(z) & 0\end{bmatrix}=\begin{bmatrix}\mathbf{e}(z) & 0\end{bmatrix}S_{\varepsilon_i}(z) \tag{7.5}$$

for some function S_{ε_i} such that

$$\begin{bmatrix} P_{\varepsilon_i} & G(w)^{-*}\left(E_{\varepsilon_i}-M_{\varepsilon_i}S_{\varepsilon_i}(w)^*\right) \\ \left(E^*_{\varepsilon_i}-S_{\varepsilon_i}(z)M^*_{\varepsilon_i}\right)G(z)^{-1} & \frac{I_{p+dn}-S_{\varepsilon_i}(z)S_{\varepsilon_i}(w)^*}{1-\langle z,w\rangle}\end{bmatrix}\succeq 0. \tag{7.6}$$

All the functions S_{ε_i} are of the class $\mathscr{S}_d^{(p+dn)\times(q+n)}$ (since the kernels $\frac{I_{p+dn}-S_{\varepsilon_i}(z)S_{\varepsilon_i}(w)^*}{1-\langle z,w\rangle}$ are positive definite on $\mathbb{B}^d\times\mathbb{B}^d$) and thus, using the arguments from the proof of Theorem 6.7, one can find a function $S_0\in\mathscr{S}_d^{(p+dn)\times(q+n)}$ and a subsequence of $\{\varepsilon_i\}$ (which still will be denoted by $\{\varepsilon_i\}$) such that

$$\lim_{i\to\infty}S_{\varepsilon_i}(z)=S_0(z)$$

and convergence is uniform on compact subsets of $\mathbb{B}^d$. Let

$$S_0=\begin{bmatrix}S & S_1\\ S_2 & S_3\end{bmatrix}:\begin{bmatrix}\mathbb{C}^q\\ \mathbb{C}^n\end{bmatrix}\to\begin{bmatrix}\mathbb{C}^p\\ \mathbb{C}^{dn}\end{bmatrix} \tag{7.7}$$

be the partition of the function S_0 into four blocks of the indicated sizes. Upon taking the limit in (7.5) as $i\to\infty$ and taking into account (7.7), we get

$$x(z)=\mathbf{e}(z)S(z). \tag{7.8}$$

Now we multiply the kernel in (7.6) by $[I_{n+p}\quad 0]$ on the left, by $[I_{n+p}\quad 0]^*$ on the right (in other words we delete the dn bottom rows and the dn right columns in (7.6)) and pass to the limit as $i\to\infty$ in the resulting inequality. On account of (7.7), we get

$$\begin{bmatrix} P & G(w)^{-*}\left(E-MS(w)^*\right) \\ \left(E^*-S(z)M^*\right)G(z)^{-1} & \frac{I_p-S(z)S(w)^*-S_1(z)S_1(w)^*}{1-\langle z,w\rangle}\end{bmatrix}\succeq 0.$$

But the last inequality clearly implies

$$\widehat{P}_S(z,w) = \begin{bmatrix} P & G(w)^{-*}\,(E - MS(w)^*) \\ (E^* - S(z)M^*)\,G(z)^{-1} & \frac{I_p - S(z)S(w)^*}{1-\langle z,w\rangle} \end{bmatrix} \succeq 0. \tag{7.9}$$

Thus, x admits a factorization (7.8) with a function S subject to (7.9). This completes the proof. □

Remark 7.1. Note that Theorem 6.6 is a consequence of Theorems 6.8 and 6.3; it looks much more reasonable to derive a more general Theorem 6.6 from a particular case covered by Theorem 6.3. In the current situation, we cannot do that, since the proof of Theorem 6.3 relies on Theorem 6.6.

In any event, Theorem 6.3 shows that Problem 1.7 reduces to Problem 6.2 which, in fact, is an interpolation problem for functions in the class $\mathscr{S}_d^{p\times q}$. It can be reformulated in a slightly different form in terms of reproducing kernel Hilbert spaces (we refer to [15] for main definitions and especially, for reproducing kernel approach to interpolation). Here we recall the fundamental result of Aronszajn [2] which states that for every positive kernel K there is a unique reproducing kernel Hilbert space $\mathscr{H}(K)$ with K as its reproducing kernel, and the following result which goes back to [7].

Lemma 7.2. *Let $K(z,w)$ be a $\mathbb{C}^{p\times p}$-valued kernel on $\Omega\times\Omega$, let $F(z)$ be a $\mathbb{C}^{p\times n}$-valued function on Ω and let $P\in\mathbb{C}^{n\times n}$. Then the kernel $\begin{bmatrix} P & F(w)^* \\ F(z) & K(z,w)\end{bmatrix}$ is positive definite on Ω if and only if*

$$P \geqslant 0, \quad K(z,w) \succeq 0 \;\; (z,w\in\Omega)$$

and for every $x\in\mathbb{C}^p$, the vector function $F(z)x$ belongs to the reproducing kernel Hilbert space $\mathscr{H}(K)$ and satisfies

$$\|Fx\|^2_{\mathscr{H}(K)} \leqslant x^*Px.$$

The latter result is equivalent to that in [7, Theorem 2.2] in case when $p=n=1$. The general (even operator-valued case) can be proved using much the same arguments (see e.g., [12, Lemma 2.1]).

For a function $S\in\mathscr{S}_d^{p\times q}$, the kernel $K_S(z,w) = \frac{I_p - S(z)S(w)^*}{1-\langle z,w\rangle}$ is positive on $\mathbb{B}^d$ (by definition) and then, there is a unique reproducing kernel Hilbert space (which will be referred below as to $\mathscr{H}(S)$) with K_S as its reproducing kernel. Making use of Lemma 7.2, we can reformulate Problem 6.2 in the following way:

Problem 7.3. Given matrices $P, T_1, \ldots, T_d \in \mathbb{C}^{n\times n}$, $E \in \mathbb{C}^{n\times p}$ and $M \in \mathbb{C}^{n\times q}$, subject to the Stein identity (1.3), find all the functions $S \in \mathscr{S}_d^{p\times q}$ such that for every $x \in \mathbb{C}^n$, the function

$$B_x(z) := (E^* - S(z)M^*)\left(I_n - \sum_{j=1}^{d} z_i T_i^*\right)^{-1} x \text{ belongs to the space } \mathscr{H}(S)$$

and satisfies

$$\|B_x\|^2_{\mathscr{H}(S)} \leqslant x^* P x.$$

The latter problem can be considered as a multivariable matricial analogue of the Abstract Interpolation Problem introduced in [21] (see also [22,25]) for Schur functions (i.e., for the case when $d = 1$). Note that inequality (6.2) is, in fact, Potapov's fundamental matrix inequality corresponding to Problem 7.3 (see [26] for the origins and [25] for general overview of the Potapov's approach to interpolation problems).

All the solutions S of Problem 7.3 (in case when P is positive definite) are parametrized by the linear transformation (6.25). It remains to clarify what interpolation conditions in Problem 7.3 mean in terms of values of S and or of its partial derivatives. This question turns out to be quite difficult (especially in case when the matrices $T_1, \ldots, T_d$ do not commute); it lies far beyond the framework of the present paper and will be treated elsewhere.

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